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# Electron–Positron Interaction in Jellium: Modification of the Perturbed Hypernetted-Chain Approach

H. Stachowiak[a] and E. Boroński[b]

[a]W. Trzebiatowski Institute for Low Temperature and Structure Research
Polish Academy of Sciences
P.O. Box 1410, 50-950 Wrocław 2, Poland
[b]Institute of Physics, University of Opole, Oleska 48, 45-052 Opole, Poland

The approach of Kahana to the electron–positron interaction in an electron gas contains the superfluous assumption that electron scattering on the positron can occur only to momentum states lying outside the Fermi sphere. The perturbed hypernetted-chain approach avoids that assumption, but self-consistency was achieved only in the Born approximation. In the present work a modification of perturbed hypernetted-chain approach allowed to reach self-consistency also at the Kohn–Sham level, at least for $1 \leq r_s \leq 3.5$. The electron–positron correlation functions obtained in this way are compared to figures resulting from other approaches.

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## 1. Introduction

Many works have been devoted to the theory of the electron–positron interaction in an electron gas (for reviews cf. [1, 2]). The differences of annihilation rates between various calculations reach about 15%. The approaches to this problem can be divided into deterministic and probabilistic (i.e. basing on Monte Carlo type calculations). We will concentrate on deterministic ones.

The deterministic approach of Kahana [3] (cf. also [4]) allows multiple scattering of electrons on the positron. Scattering, however, is allowed only to momentum states outside the Fermi sphere. This is an assumption which imposes additional restraints on the wave function. They do not follow from physical principles since here the antisymmetry of the wave function is a sufficient requirement. As pointed out by Lowy and Jackson [5], in the case of multiple scattering free space will appear inside the Fermi sea to which scattering can occur. Let us mention here that some deficiencies occurring in the original Kahana approach

have been removed in the calculations of Rubaszek and Stachowiak [6] which are self-consistent, include the exchange-correlation correction and base on the exact solution of the two-particle equations.

The approach of Lantto [7] (cf. also Ref. [8]) applies the methods of the theory of liquids, in particular the Fermi hypernetted-chain (FHNC) approximation. However, the Jastrow type trial function used in the calculations leaves much to be desired, since it does not allow different electronic states to scatter on the positron in a way depending on their momentum. Besides the calculations do not include three-particle correlations. In the density functional formalism these correlations lead to the exchange-correlation correction in the potential. Its importance for positron lifetime calculations has been demonstrated many times [9, 6, 10, 1]. Indeed, if the exchange-correlation effect is neglected, the electrons scatter on a partially screened positron, even at large values of $r_s$ because the exchange-correlation hole is not subtracted from the electron density. This makes the positron annihilation rate to fall below the value for spin-averaged positronium, which is an unphysical result. The Monte Carlo calculations of Fraser confirm this expectation [11]. The more sophisticated Monte Carlo studies of Boroński basing on the same form of the trial function yield somewhat different figures, but their results remain unphysical for large values of $r_s$ [12]. In agreement with expectations Boroński by including three-particle correlations into the trial function greatly improved the annihilation rates by getting rid of their unphysical features to a large degree.

Nevertheless, the results of Lantto have been parameterized (at least in the metallic range) by Boroński and Nieminen [13]. Their formula agrees remarkably well with experiment. It will be labelled BN in the following.

Values of the annihilation rates lower than those of Rubaszek and Stachowiak have been obtained by Stachowiak and Lach [10, 14] using the perturbed hypernetted chain (PHNC) approach. The method consists in considering the wave function of the system in the form of a Jastrow type function augmented by terms allowing different scattering on the positron of different electronic states. The multiplicative term in the wave function was chosen as the density amplitude of electrons screening the positron. This last was computed according to the equation proposed by Gondzik and Stachowiak [9].

Since the multiplicative term includes most of the effect of $e^+$–$e^-$ interaction, one can hope that multiple scattering can be omitted while perturbing the Jastrow type states. This allows to solve the one positron–one electron Kohn–Sham-like equation in a self-consistent Born approximation.

The annihilation rates obtained in this way are intermediary between those of Arponen and Pajanne [15] and Rubaszek and Stachowiak on one side and BN on the other.

Let us note that Lantto's calculations do not exceed $r_s = 5$. Since it should be expected that for large values of $r_s$ their results will fall unphysically below

the value for spin-averaged positronium, it is logical to assume that their better agreement with experiment is due to the fact that the approaches of Refs. [5, 6, 15] and [10] are unable to cope with some effects, so they overestimate the annihilation rates. The approach of Lantto does not cope either, but accidentally the errors it introduces lead for $r_s \leq 5$ to annihilation rates closer to the correct value than those obtained in other deterministic approaches.

As concerns the PHNC screened potential of the $e^+$–$e^-$ interaction, it is not self-consistent in the Kohn–Sham sense, i.e. when introduced in the Kohn–Sham-like equation it does not lead to the PHNC electron distribution. Our aim in the present work is to modify the equation of Gondzik and Stachowiak in such a way as to obtain a self-consistent potential by performing PHNC calculations. Unlike in the original PHNC approach of Refs. [10, 14] this potential — when introduced in the Kohn–Sham-like equations describing the two-particle $e^+$–$e^-$ interaction — would lead to an electron distribution generating the same potential.

The way of achieving this aim has been proposed in Ref. [16]. In the present work we perform calculations using this formalism. A numerical program was elaborated for determining the optimal values of the three parameters assumed in the factor $p(s)$ of Ref. [16] in order to obtain the self-consistency.

## 2. The two-particle approximation

In this work we will assume consequently that the interaction of electrons in an electron gas with the positron consists in the interaction of particular electronic states with the positron, and momentum conservation occurs in this two-particle system. This is the reason of the usefulness of positron annihilation in studies of the electronic structure.

The wave function of the jellium-one positron system is assumed as a Slater determinant built of functions $\psi_{\boldsymbol{k}\sigma}(\boldsymbol{r}_\mathrm{e}, \boldsymbol{r}_\mathrm{p})$. Here $\boldsymbol{r}_\mathrm{e}$ and $\boldsymbol{r}_\mathrm{p}$ are electron and positron coordinates, respectively. The electron spin index $\sigma$ will be omitted unless necessary. The functions $\psi_{\boldsymbol{k}}$ describe the scattering of the electron plane wave on the screened positron and obey the equation (in Hartree atomic units)

$$\left[-\tfrac{1}{2}\nabla_\mathrm{e}^2 - \tfrac{1}{2}\nabla_\mathrm{p}^2 + V(|\boldsymbol{r}_\mathrm{e} - \boldsymbol{r}_\mathrm{p}|)\right]\psi_{\boldsymbol{k}} = \frac{k^2}{2}\psi_{\boldsymbol{k}}. \tag{1}$$

The screened Coulomb potential $V(s)$ will be computed self-consistently under the assumption that it takes the local Kohn–Sham form.

After introducing reduced coordinates we find [10, 16] that the wave function of the system can be presented in the form of the Slater determinant built of functions

$$\psi_{\boldsymbol{k}}(\boldsymbol{s}) = \frac{1}{\sqrt{\Omega}}\left[\exp(\mathrm{i}\boldsymbol{k}\boldsymbol{s}) + \exp(\mathrm{i}\tfrac{\boldsymbol{k}}{2}\boldsymbol{s})\sum_{l=0}^{l_M}(2l+1)\mathrm{i}^l\beta_l(\tfrac{k}{2}, s)P_l(\cos\vartheta)\right], \tag{2}$$

where $\boldsymbol{s} = \boldsymbol{r}_\mathrm{e} - \boldsymbol{r}_\mathrm{p}$ and $\beta_l$ are obtained by solving Eq. (1) in reduced coordinates, i.e.

$$\left[-\tfrac{1}{2}\nabla^2 + \tfrac{1}{2}V(s)\right] u_{\boldsymbol{k}} = \frac{k^2}{8} u_{\boldsymbol{k}}. \tag{3}$$

$\Omega$ is the volume of the sample. $u_{\boldsymbol{k}}$ is obtained in the form

$$u_{\boldsymbol{k}}(\boldsymbol{s}) = \frac{1}{\sqrt{\Omega}} \left[ \exp(\mathrm{i}\tfrac{\boldsymbol{k}}{2}\boldsymbol{s}) + \sum_{l=0}^{l_M} (2l+1)\mathrm{i}^l \beta_l(\tfrac{k}{2}, s) P_l(\cos\vartheta) \right], \tag{4}$$

where $\vartheta$ is the angle between $\boldsymbol{s}$ and $\boldsymbol{k}$. $l_M$ indicates the number of partial waves used in the computations. In this work we will put $l_M = 2$. Let us also define $b_l(\frac{k}{2}, s)$ by means of the equation

$$\beta_l(\tfrac{k}{2}, s) = \exp(\mathrm{i}\delta_l \tfrac{k}{2}) b_l(\tfrac{k}{2}, s) - j_l(\tfrac{k}{2}s), \tag{5}$$

$\delta_l$ indicates phase shifts, $j_l$ the appropriate Bessel function and $b_l$ satisfies the relation

$$R_l(\tfrac{k}{2}, s) = (2l+1)\mathrm{i}^l \exp(\mathrm{i}\delta_l \tfrac{k}{2}) b_l(\tfrac{k}{2}, s), \tag{6}$$

where $R_l$ is the solution of Eq. (3).

In the present work we will use the Slater determinant written in the form

$$\Psi(\boldsymbol{s}_1, \ldots, \boldsymbol{s}_N) = \prod_{i=0}^{N} w(s_i) \begin{vmatrix} \varphi_1(\boldsymbol{s}_1) & \varphi_1(\boldsymbol{s}_2) & \ldots & \varphi_1(\boldsymbol{s}_N) \\ \varphi_2(\boldsymbol{s}_1) & \varphi_2(\boldsymbol{s}_2) & \ldots & \varphi_2(\boldsymbol{s}_N) \\ \ldots & \ldots & \ldots & \ldots \\ \varphi_N(\boldsymbol{s}_1) & \ldots & \ldots & \varphi_N(\boldsymbol{s}_N) \end{vmatrix}, \tag{7}$$

where $\boldsymbol{s}_i = \boldsymbol{r}_i - \boldsymbol{r}_{\mathrm{p}}$ and

$$\varphi_{\boldsymbol{k}}(s) = \frac{1}{\Omega^{1/2}} [\mathrm{e}^{\mathrm{i}\boldsymbol{k}\boldsymbol{s}} + \mathrm{v}_{\boldsymbol{k}}(\boldsymbol{s})]. \tag{8}$$

In PHNC $v_{\boldsymbol{k}}(\boldsymbol{s})$ is computed in the self-consistent Born approximation.

Since all electronic states are attracted by the positron, we can describe approximately this attraction by one function $w(s)$ putting

$$\psi_{\boldsymbol{k}}(\boldsymbol{s}) = w(s)\varphi_{\boldsymbol{k}}(\boldsymbol{s}) \tag{9}$$

and hope that the function $v_{\boldsymbol{k}}(\boldsymbol{s})$ of Eq. (8) is small provided the function $w(s)$ includes most of the effect of the interaction.

In the case of a weak nonorthogonality of the wave functions $\varphi_{\boldsymbol{k}}$, we can write the electron density in the form [10]:

$$\rho(s) = w^2(s)\rho_0 + \delta\rho^3(s) - \delta\rho^1(s) - \delta\rho^2(s) = w^2(s)\rho_0 + \delta\rho(s). \tag{10}$$

According to PHNC we have

$$\delta\rho^3(s) - \delta\rho^2(s) = \frac{w^2(s)}{2\pi^4 s} \int_0^\infty \mathrm{d}q [\Phi_1(q)K_1(q) + \Phi_2(q)K_2(q)] \sin(qs), \tag{11}$$

where $K_1$ and $K_2$ are given in [10]. $\Phi_1(q)$ and $\Phi_2(q)$ obey the formulae

$$\Phi_1(q) = \frac{4\pi}{q^2}\int_0^\infty \mathrm{d}s W(s)[\sin(qs) - qs\cos(qs)], \tag{12}$$

$$\Phi_2(q) = -\frac{4\pi}{q}\int_0^\infty \mathrm{d}s s v(s)\sin(qs). \tag{13}$$

$\theta$ is the angle between $\boldsymbol{k}$ and $\boldsymbol{q}$.

$$W(s) = \frac{1}{w}\frac{\mathrm{d}w}{\mathrm{d}s}. \tag{14}$$

$v(s) = V(s) - V_0(s)$ and is unknown.

Let us note that the total electron density around the positron is expressed partly in terms of the unknown function $\Phi_2(q)$ defined by Eq. (13). This function in real space corresponds to the unknown correction $v(s)$ to the electron–positron potential.

Our aim is to express $w(s)$ in a suitable form which at the same time would be sufficiently flexible. In Ref. [10] $w(s)$ was approximated as the density amplitude obtained from the HNC equation of Gondzik and Stachowiak (Ref. [9])

$$[-\nabla^2 + V_0(\boldsymbol{s})]w(\boldsymbol{s}) = 0 \tag{15}$$

with the potential

$$V_0(\boldsymbol{s}) = -\frac{1}{s} + \rho_0\int \mathrm{d}\boldsymbol{s}'\frac{w^2(s')-1}{|\boldsymbol{s}-\boldsymbol{s}'|} + \{V_{\mathrm{HL}}[w^2(s)\rho_0] - V_{\mathrm{HL}}(\rho_0)\}, \tag{16}$$

where the HNC electron density is given by $\rho(\boldsymbol{s}) = w^2(\boldsymbol{s})\rho_0$. The subscript HL means that we choose the Hedin–Lundqvist form of the exchange-correlation correction [17].

In our case it would be particularly desirable if $w(s)$ led to a total screening charge neutralizing the charge of the positron. Such a requirement is satisfied by the solution of Eq. (15) with the potential

$$V_0(\boldsymbol{s}) = -\frac{1}{s} + \rho_0\int \mathrm{d}\boldsymbol{s}'\frac{w^2(s')-1}{|\boldsymbol{s}-\boldsymbol{s}'|} + p(s)\{V_{\mathrm{HL}}[w^2(s)\rho_0] - V_{\mathrm{HL}}(\rho_0)\}. \tag{17}$$

We estimate that a sufficient flexibility of the approach will be provided by $p(s)$ in the form

$$p(s) = A\mathrm{e}^{-Bs} + C. \tag{18}$$

In the original form of the equation of Gondzik and Stachowiak [9] $p(s)$ is equal to 1.

The form (17) of the potential $V_0(s)$ does not mean any assumption concerning the exchange-correlation potential. This is just a way of obtaining a parameter dependent function $w(s)$. The way of computing $v(s)$ is given in [10].

## 3. Comparison of the two electron distributions

The density $\rho(s)$ depends on the functions $w(s)$ and $v_{\boldsymbol{k}}(s)$ and is expressed by the formula (10). However, the functions $v_{\boldsymbol{k}}(s)$ depend on whether we compute them according to PHNC or using the potential $V(s)$ in Eq. (1). In this last case, applying Eqs. (2), (5) and (8) we have

$$v_{\boldsymbol{k}}(\boldsymbol{s}) = \exp(\mathrm{i}\tfrac{\boldsymbol{k}}{2}\boldsymbol{s}) \sum_{l=0}^{l_N} (2l+1)\mathrm{i}^l \gamma_l(\tfrac{k}{2}, s) P_l(\cos\vartheta), \tag{19}$$

where we get for $l \leq l_M$

$$\gamma_l(\tfrac{k}{2}, s) = \exp(\mathrm{i}\delta_l(\tfrac{k}{2})) \frac{b_l(\frac{k}{2}, s)}{w(s)} - j_l(\tfrac{k}{2}s) \tag{20}$$

and for $l > l_M$

$$\gamma_l(\tfrac{k}{2}, s) = \left[\frac{1}{w(s)} - 1\right] j_l(\tfrac{k}{2}s). \tag{21}$$

While $l$ increases, the function $j_l(\frac{k}{2}s)$ starts to become big for higher and higher values of $s$ where the coefficient $\frac{1}{w(s)} - 1$ in Eq. (21) is small. This limits the value of $l_N$. In actual computations we will not use values of $l$ bigger than 2.

In the expression (10) for $\rho(s)$ only the part $\delta\rho^3(s) - \delta\rho^2(s)$ depends on $v_{\boldsymbol{k}}(s)$ (cf. [10]). Therefore, it could be different depending on whether we compute it using the formula (11). We obtain in this way the function $f(s)$, or whether we use for this purpose the formula (19) for $v_{\boldsymbol{k}}(s)$, we obtain in this case the function $g(s)$. If $f(s)$ and $g(s)$ differ strongly from each other, this means that the assumptions underlying the PHNC approach are not quite satisfied. A function $w(s)$ leading to similar functions $f(s)$ and $g(s)$ is more satisfactory than one providing very different functions. Equality of $f(s)$ and $g(s)$ means that we indeed obtained the solution of the many-body problem within the approximations used in this work, in particular assuming the wave function of the system in the form of a Slater determinant built of functions (2) and the electron distribution according to the formula (10).

### *3.1. Computation of $g(s)$*

We have

$$g(s) = \delta\rho^3_{\mathrm{KS}}(s) - \delta\rho^2_{\mathrm{KS}}(s), \tag{22}$$

where the subscript KS (Kohn–Sham) indicates that in performing computations the form (19) of $v_{\boldsymbol{k}}(\boldsymbol{s})$ is used.

We have

$$\delta\rho^3_{\mathrm{KS}}(s) = \frac{2w^2(s)}{\pi^2} \sum_{l=0}^{l_N} (2l+1) \int_0^{k_{\mathrm{F}}} k^2 \mathrm{d}k \mathrm{Re}\left[\gamma_l(\tfrac{k}{2}, s)\right] j_l(\tfrac{k}{2}s) \tag{23}$$

and

$$\delta\rho^2_{\mathrm{KS}}(s) = \frac{2w^2(s)}{\pi^3} \sum_{l=0}^{l_N} (2l+1) \int_0^{k_{\mathrm{F}}} \mathrm{d}k' \int_0^{\infty} \mathrm{d}s' \mathrm{Re}\left[\gamma_l(\tfrac{k'}{2}, s')\right] K_l(k', s', s). \tag{24}$$

The function $K_l(k', s', s)$ is universal, i.e. it is independent of the physical ingredient $\gamma_l(\frac{k}{2}, s)$. This is of great help in numerical computations.

### *3.2. Comparison of $f(s)$ and $g(s)$*

The PHNC potential is self-consistent in the Born approximation. Our calculations will show to be consistent if solving exactly the Kohn–Sham-like Eqs. (1)

with this potential will lead approximately to the same electron distribution around the positron. In other words, $f(s)$ and $g(s)$ should be close to each other. Since we cannot expect that these two functions will be identical, we must assume some numerical quantity which would express by means of a single number the similarity of the two functions. We believe that it is crucial that both functions generate the same contribution to the potential. Assuming that the self-consistent Born approximation predicts an electron density distribution around the positron equal $\rho_1(s)$ and a potential $V_1(s)$ while the exact solution of the Kohn–Sham equations with the same potential gives an electron distribution $\rho_2(s)$ which generates a potential $V_2(s)$ we find it logical to minimize with regard to $p(s)$ the integral

$$\Delta[p(s)] = \int s^2 \mathrm{d}s [V_2(s)\rho_2(s) - V_1(s)\rho_1(s)]^2. \tag{25}$$

We have

$$\rho_2(s) = \rho_1(s) + g(s) - f(s) \tag{26}$$

and

$$V_i(s) = -\frac{1}{s} + \int \mathrm{d}\boldsymbol{s}' \frac{\rho_i(s') - \rho_0}{|\boldsymbol{s} - \boldsymbol{s}'|} + V_{\mathrm{HL}}(\rho_i, s) - V_{\mathrm{HL}}(\rho_0). \tag{27}$$

This gives

$$V_2(s) = V_1(s) + \int \mathrm{d}\boldsymbol{s}' \frac{g(s') - f(s')}{|\boldsymbol{s} - \boldsymbol{s}'|} + V_{\mathrm{HL}}(\rho_2, s) - V_{\mathrm{HL}}(\rho_1, s) \tag{28}$$

and

$$\Delta[p(s)] = \int s^2 \mathrm{d}s \{[V_2(s) - V_1(s)]\rho_2(s) + V_1(s)[g(s) - f(s)]\}^2. \tag{29}$$

## 4. Computations and results

It is obvious that calculations should be performed for different densities of the electron gas characterized by the parameter $r_s$.

The dimensions of the electron gas are infinite. However, in order to perform calculations we must fix a radius of the screening cloud, assuming that outside this radius the electron gas is not disturbed by the positron. We decided to characterize this radius by a coefficient $D$ such that the radius of the screening cloud $s_{\max}$ is defined as

$$s_{\max} = R + D(s^0_{\max} - R), \tag{30}$$

where $R$ was put equal to 3 and $s^0_{\max} = 17.04$.

For a given value of $r_s$ calculations were performed for different values of $D$. For each such value we found the parameters $A$, $B$, and $C$ of the function $p(s)$ for which $\Delta[p(s)]$ reaches minimum. Unfortunately, we can investigate for technical reasons only discrete points in the three-dimensional space formed by the values of $A$, $B$, and $C$. Moreover, local minima occur in the function $\Delta[p(s)]$, which can be misleading.

Let us demonstrate the results on the example of the very typical electron density corresponding to $r_{\mathrm{s}} = 2$. The lowest value of $\Delta[p(s)]$ equal to $0.2877 \times 10^{-5}$

was obtained for $D = 1.53$ and $p_M(s)$ defined by the parameters $A = 1.8$, $B = 1.3$ and $C = 1.2577$. In Fig. 1 we show the functions $g(s)$ and $f(s)$ for $p_0(s)$ and $p_M(s)$ where we label $p_0(s)$ the function $p(s)$ with $A = 0$, $B = 0$ and $C = 1$. We can appreciate the degree of self-consistency reached in our calculations.

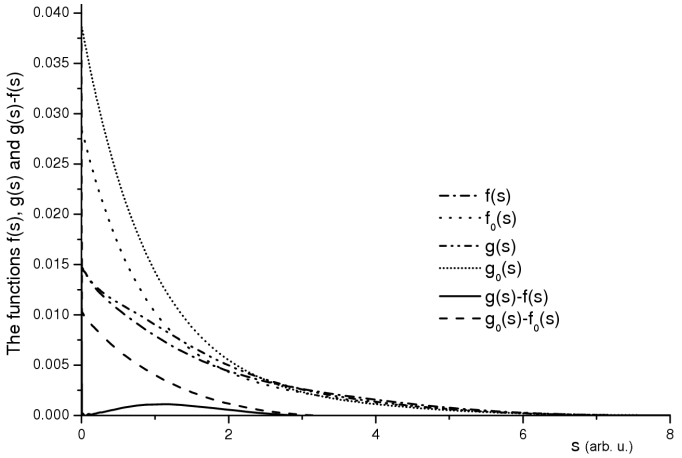


Fig. 1. The functions $f(s)$ and $g(s)$ correspond to the minimal value of $\Delta[p(s)]$ obtained at $r_s = 2$ and $D = 1.53$ for $p(s) = p_M(s)$ defined by $A = 1.8$, $B = 1.3$ and $C = 1.2577$. The figure shows also the functions $f_0(s)$, $g_0(s)$ and $g_0(s) - f_0(s)$ corresponding to $p_0(s)$, i.e. while $A = 0$, $B = 0$, and $C = 1$.

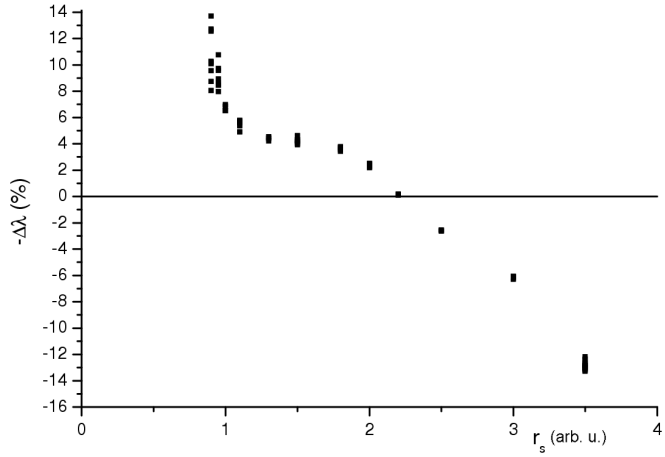


Fig. 2. The change of the annihilation rate in percent for different values of $r_s$ (keep attention to the sign of $\Delta\lambda$ where $\Delta\lambda$ is the change of the annihilation rate).

The final results are collected in Fig. 2. The decrease in the annihilation rate is shown for different values of $r_s$. The annihilation rate is not always well defined.

The same very low values of $\Delta[p(s)]$ correspond to markedly different annihilation rates. For $r_s = 0.9$ the spreading of their values is particularly high, moreover self-consistency is not satisfactory. Therefore, calculations for lower values of $r_s$ cannot be hoped to be reliable. Also calculations for $r_s > 3.5$ did not lead to self-consistency.

## 5. Conclusions

The purpose of this work was to develop a formalism which would describe self-consistently the screening of a positron in an electron gas.

In comparison with the approach of Kahana (the approach of Arponen and Pajanne leads to similar annihilation rates) our approach does not introduce the superfluous assumption of forbidding electrons to scatter to momentum states inside the Fermi sphere. In comparison with the approach of Lantto our approach includes momentum dependence of the scattering and three-particle correlations. In comparison with PHNC our electron distributions are self-consistent not only within the Born approximation but also while solving the Kohn–Sham-like equations exactly.

In this work we were able to achieve self-consistency only for $0.9 \leq r_s \leq 3.5$. We do not know to what extent this is due to the form of the modified equation of Gondzik and Stachowiak or to the PHNC formalism applied in the computations.

It is necessary to underline that we chose as criterion of self-consistency the equality of the PHNC and Kohn–Sham distributions of the potential energy of the screening cloud. This criterion leads to equality of the screening cloud distributions only for $r_s \geq 1$.

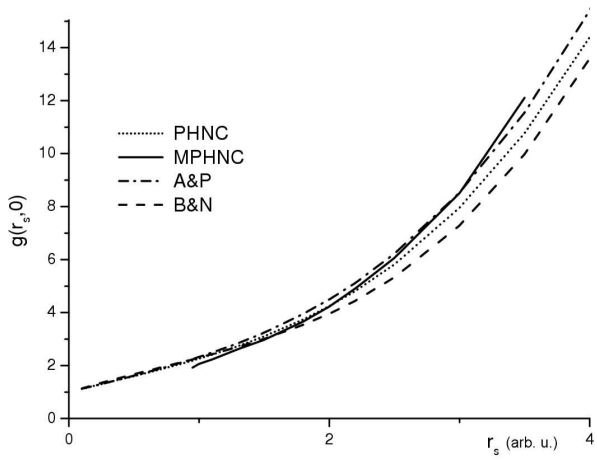


Fig. 3. The electron–positron correlation function $g(r_s, 0)$ according to different approaches: BN [13] (dashed line), PHNC [14] (dotted line), Arponen and Pajanne [15] (dashed-dotted line). The solid curve (MPHNC) shows the results of the present work.

In Fig. 3 the correlation function on the positron $g(r_s, 0)$ obtained in our work is shown and compared to the curves of Arponen and Pajanne [15], of Boroński and Nieminen [13] and of Stachowiak and Lach [10, 14].

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